

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 219 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.91e-01

Confidence level: 6.62e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Molinate</div> <div>Measured: 83.2</div> <div>Predicted: 219</div>	<div>Image not found</div> <div>EPTC</div> <div>Measured: 240</div> <div>Predicted: 204</div>	<div>Image not found</div> <div>Propachlor</div> <div>Measured: 263</div> <div>Predicted: 246</div>
<div>Image not found</div> <div>Vernolate</div> <div>Measured: 214</div> <div>Predicted: 379</div>	<div>Image not found</div> <div>Chlordimeform</div> <div>Measured: 813</div> <div>Predicted: 340</div>	